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Accelerated Gradient Descent Methods for the Uniaxially Constrained Landau-de Gennes Model

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Abstract. This paper illustrates the efficacy of using accelerated gradient descent schemes for minimizing a uniaxially constrained Landau-de Gennes model for nematic liquid crystals. Three (alternating direction) minimization schemes are applied to a structure preserving finite element discretization of the uniaxial model: a standard gradient descent method, the "heavy-ball" method, and Nesterov's method. The performance of the schemes is measured in terms of the number of iterations required to obtain the equilibrium state, as well as the total computational time (wall time).

The numerical experiments clearly show that the accelerated gradient descent schemes reduce the number of iterations and computational time significantly, despite the hard uniaxial constraint that is not "smooth" when defects are present. Moreover, our results show that accelerated schemes are not hindered when combined with an alternating direction minimization algorithm and are easy to implement.

AMS subject classifications: 65N30, 49M25, 35J70

Key words: Liquid crystals, Landau-de Gennes, uniaxial, heavy-ball method, Nesterov's method.

1 Introduction

Liquid crystals (LCs) are important in many emerging technologies [17,28]. They are easily actuated by optical effects [8,15,20,23,57], electric/magnetic [2,10,51], and mechanical forces [7,18,50,69], which has yielded various devices, e.g., electronic shutters [22], novel types of lasers [14,24], dynamic shape control of elastic bodies [11,62], and others [31,37,58,61,63].

LC models use an order parameter that represents the statistical average of the orientation of the LC molecules [59]. The Landau-de Gennes (LdG) model is popular and

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uses a *tensor-valued* function $\mathbf{Q}$ to model the orientational state of the LC material. In particular, the eigenframe of $\mathbf{Q}$ yields information about the distribution of LC molecules. Moreover, the energy functional (of $\mathbf{Q}$) for the LC material involves an elastic contribution and a bulk potential. Equilibrium LC states are minimizers of the energy functional.

This paper is concerned with a specific variant of the LdG model where *uniaxiality* is enforced as a hard constraint (see Section 3). When defects are present, i.e., when the order parameter $\mathbf{Q}$ vanishes, this constraint is *not smooth*, which makes using standard second order methods difficult (e.g., a monolithic Newton method). Of course, standard gradient descent methods can be used and are robust, but can be extremely slow to converge to a minimizer. Therefore, we investigate alternative methods for minimizing the energy functional, so-called accelerated gradient descent methods, e.g., the "heavy-ball" method [47] and Nesterov's method [40]. Our numerical experiments clearly show that both the heavy-ball method and Nesterov method are significantly better than standard gradient descent, despite the presence of the non-smooth uniaxial constraint.

Although many numerical methods and implementations exist for the standard LdG model, e.g., [5, 6, 9, 16, 30, 49, 66, 67], to the best of our knowledge, accelerated gradient methods for LC simulations, in general, are not typically used. There are, of course, examples of accelerated methods used for other types of PDEs. For example, in [25], they consider a phase field crystal model. In that work, they establish various analytical results, including convergence guarantees for their accelerated method. However, the model we consider has an *elliptic degeneracy* (see Remark 3.2, as well as [9, 44]), which is a major analytical difficulty that does not appear in the model considered by [25]. Indeed, it is not clear how to derive a convergence guarantee that accounts for the elliptic degeneracy and the associated non-smooth constraint. Our main contribution is to demonstrate that well-known acceleration techniques are still effective in speeding up convergence to a minimizer for energy functionals that are degenerate with non-smooth constraints.

This paper is organized as follows. A review of the Landau-de Gennes model using the one constant version is presented in Section 2. The Landau-de Gennes model is reduced to the uniaxially constrained model in Section 3. A high level description of the minimization schemes is reviewed in Section 4, and then applied to minimizing the Landau-de Gennes energy in Section 5. Numerical experiments are conducted in Section 6 to illustrate the performance of the minimization schemes. We close with some remarks in Section 7.

2 The Landau-de Gennes model

We briefly review the Landau-de Gennes model [17, 55]. Let $\Omega \subset \mathbb{R}^d$, with $d = 2,3$, be the domain of the LC material (assume Ω is Lipschitz). The order parameter $\mathbf{Q}$ is a tensor-valued function $\mathbf{Q}: \Omega \to \mathbf{\Lambda}$, where

$$\mathbf{\Lambda} := \{\mathbf{A} \in \mathbb{R}^{d\times d} \,|\, \mathbf{A} = \mathbf{A}^T,\ \mathrm{tr}(\mathbf{A}) = 0\}. \tag{2.1}$$